Shortening the Insertion Time for Materials Technologies— the 21st Century Metals Challenge

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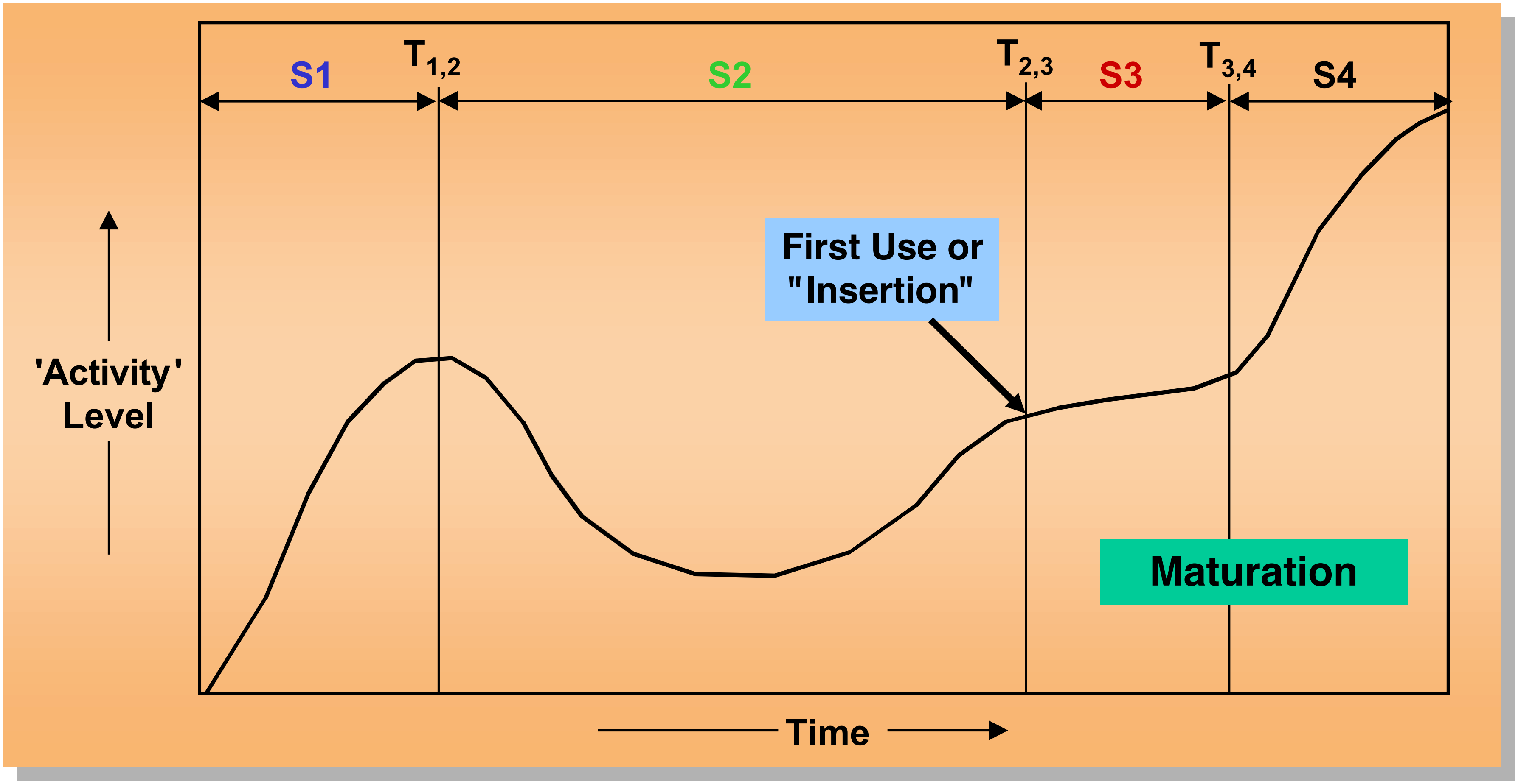
Advanced Metallics Research Group

Leo Christodoulou, Steve Wax

Observation: Historical Aerospace Material Life Cycle

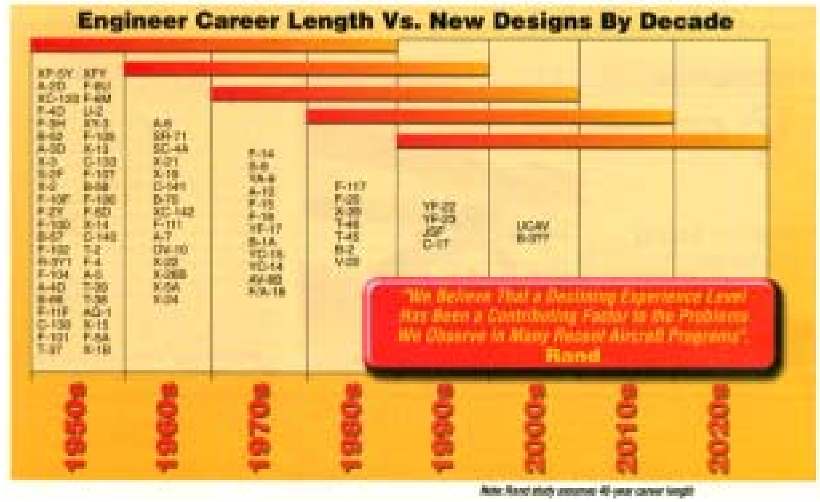


Stages

S1 = Revolutionary
S2 = Emerging
S3 = Specialty Material
S4 = Commodity Material

Aerospace Structural Materials Development: How It Happened

Adapted from Fraser, 1998; Wax, 1999



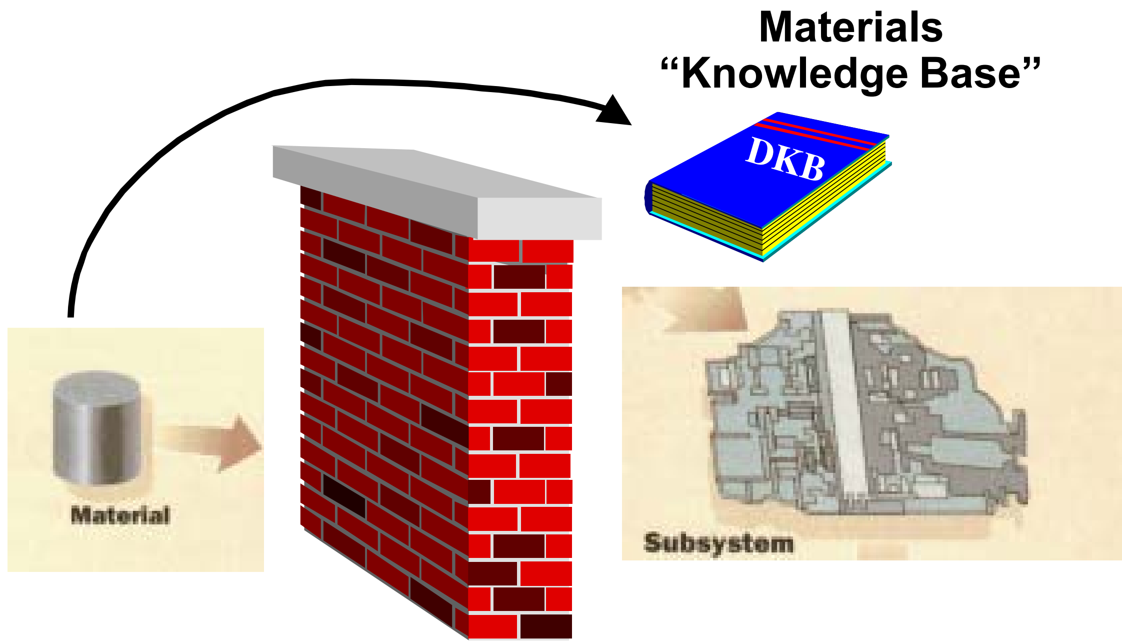
- DoD materials **transition opportunities** (systems) have drastically **reduced**
- Material development time far exceeds the **modern short product cycle**
  - iterative, empirical development of "Knowledge Base" is lengthy, data intensive, and expensive

21st Century Reality <u>Demands</u> that the Paradigm Change!

The Disconnect!

Major disconnect between materials development & components/systems engineering design

- Known alloy to reliable part ~36 months
- Steels for navy landing gear 15+ yrs
- Lightweight composites for army vehicles 15+ yrs
- Gamma titanium aluminides ~30yrs and counting
- Ceramics for engines - 30+++ ? yrs
- Evolutionary alloy changes (ship steels, superalloys, etc) ~7-10 years



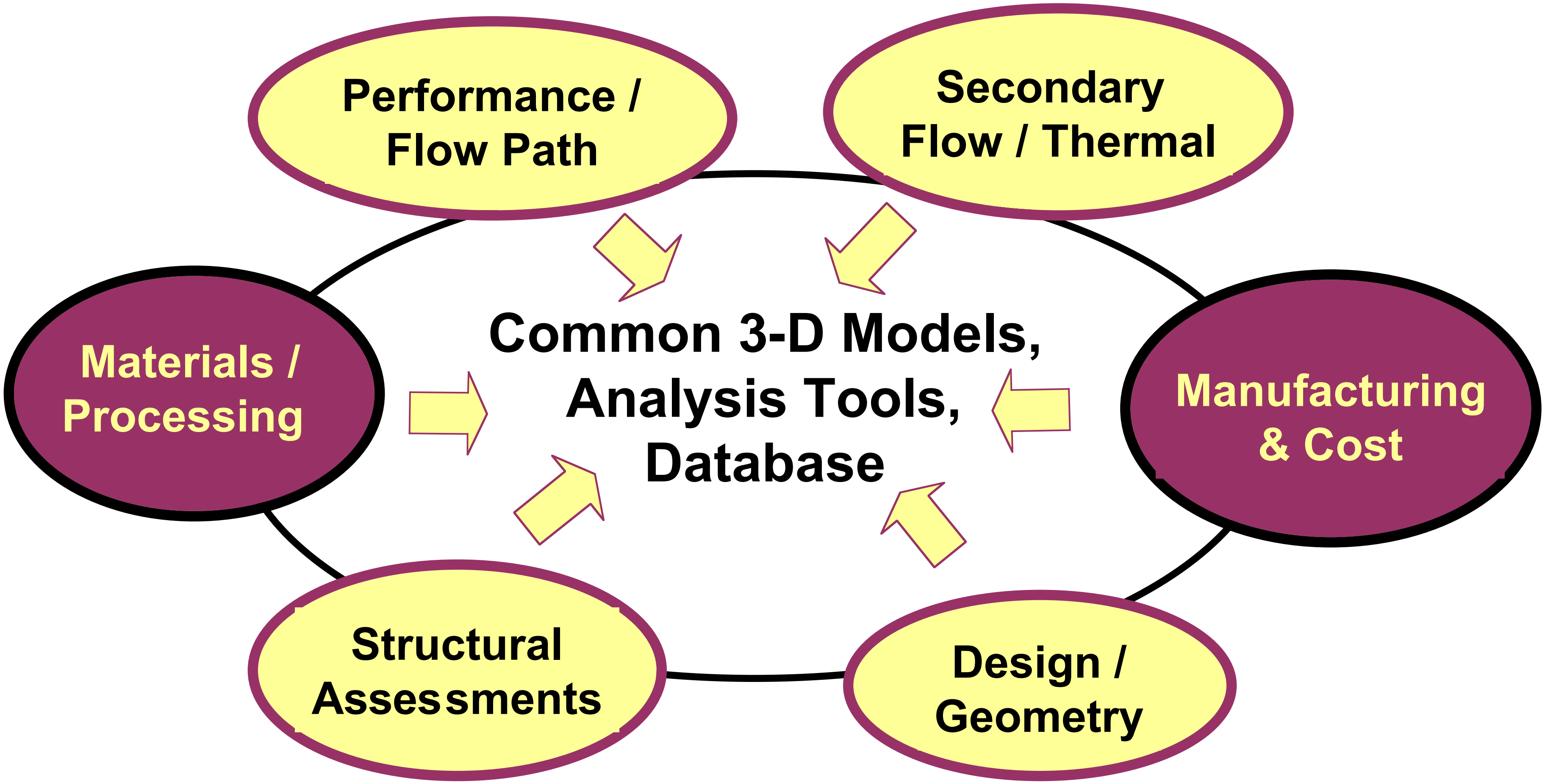
Materials Development
- Highly Empirical
- Testing Independent of Use
- Existing Models Unlinked

Engineering Design
- Materials Input from "Knowledge Base" of Data (Data Sheets, Graphs, Heuristics, Experience, etc.)
- System/Sub-System Design is Heavily Computational and Rapid
- Well Established Testing Protocols

DARPA

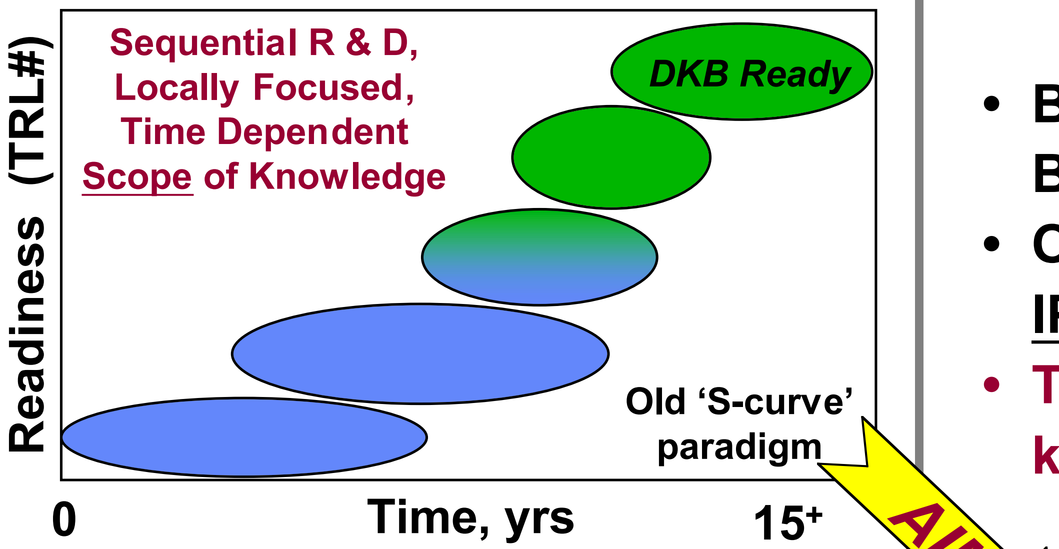
 Adapted from Wax, 1999

Integrating Materials & Processes with Engine Design



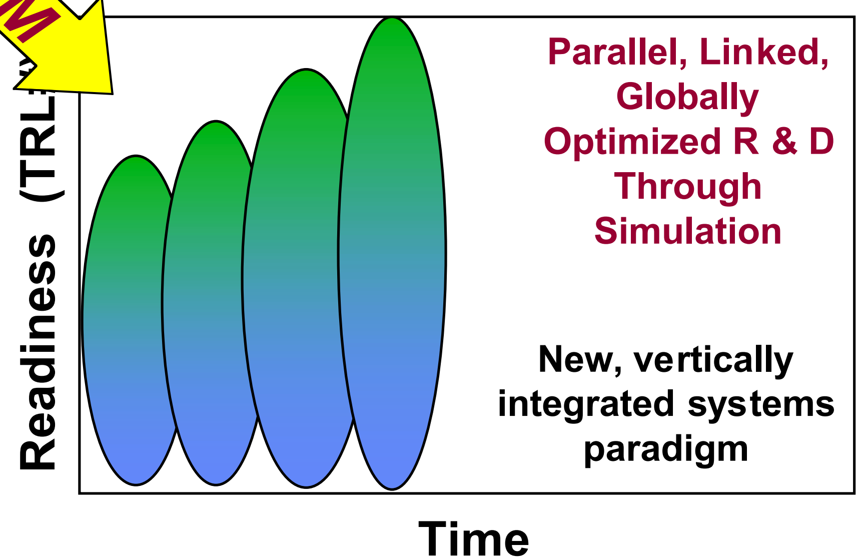
Design “development cycle”: <3 yrs	Materials & Process "cycle": 7-20 yrs

AIM Paradigm for Materials R & D

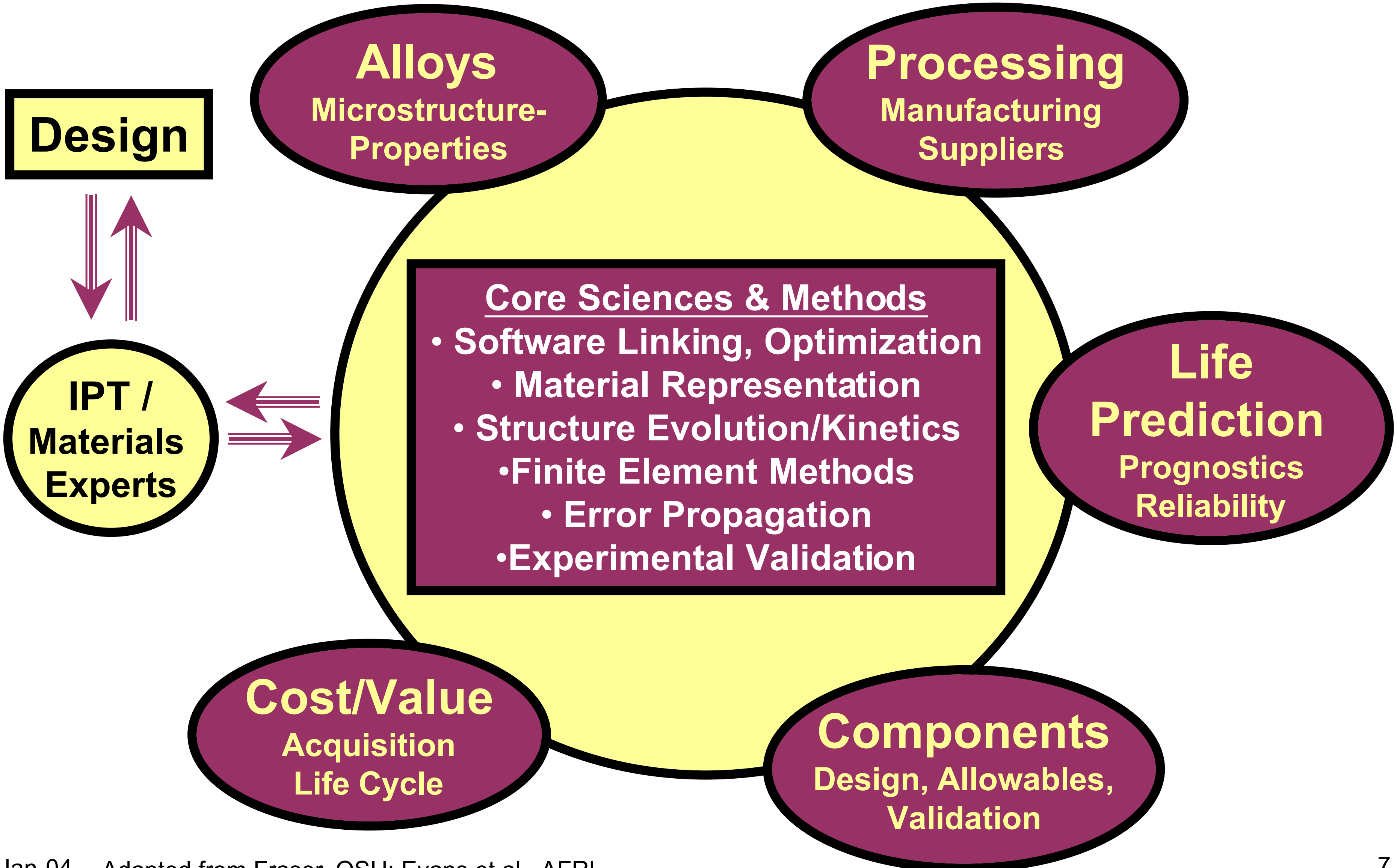


- Sequential M & P
- Optimized from heuristics
- "Designer Knowledge Base" NOT Ready Until Final Stages

- Building "Designer Knowledge Base" begins at outset
- Optimization based on <u>design IPT need</u>
- Time & effort refines <u>quality</u> of knowledge base, <u>not its scope</u>



Major Components of Designer Knowledge Base

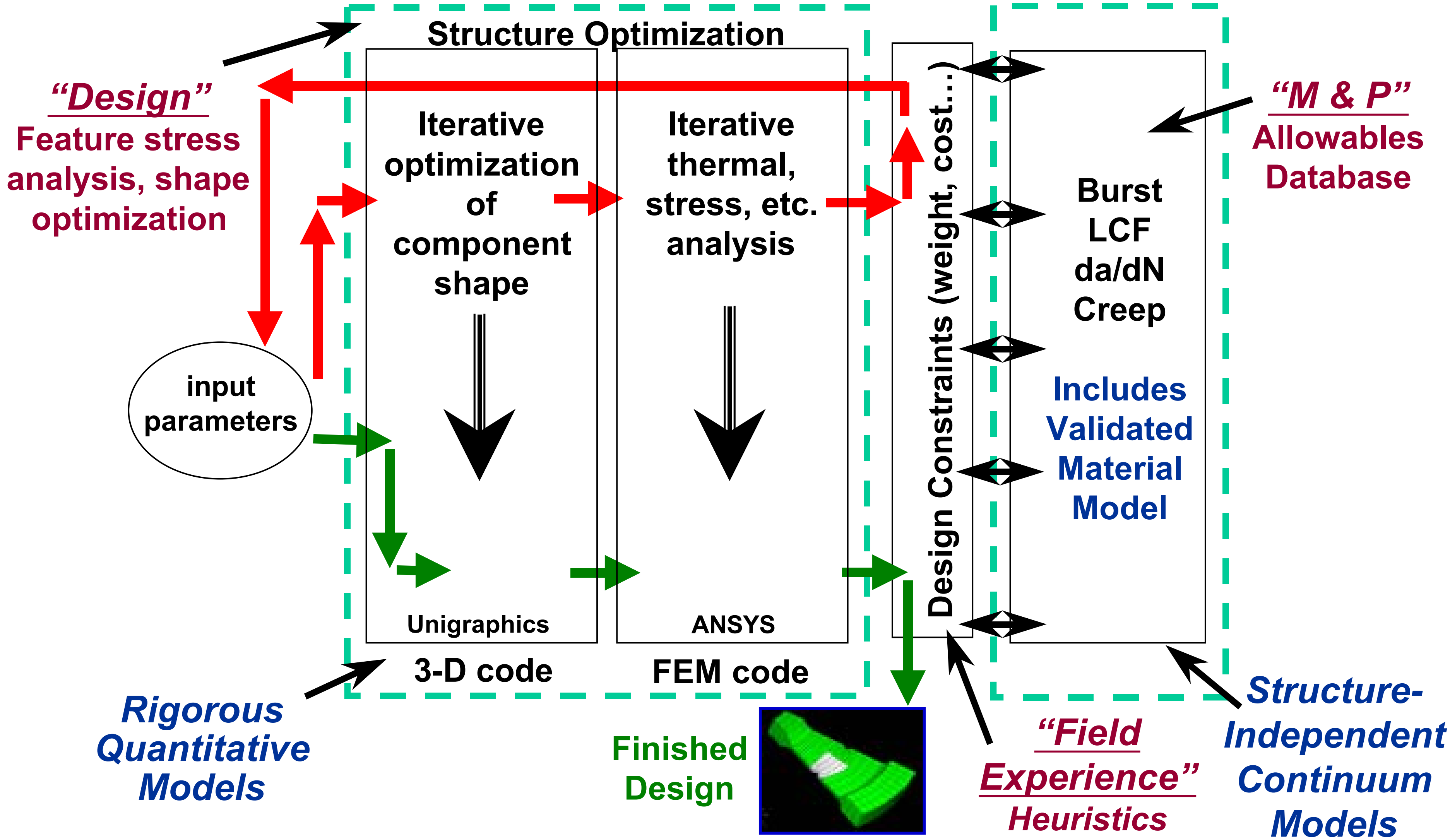


Guiding Constraints

- **A key deliverable must be a validated representation of the material and process: *designers work with representations!***
- **Structural materials design demands confidence in *control of time-dependent properties*, thus representations needed for**
  LCF, HCF, crack growth
  creep, stress rupture
  environmental degradation, stress corrosion
  friction, wear, and fretting
- ***'New material' demands rapid, validated representations*—but how?**
- **Need *ubiquitous tools* for optimization:**
  a representation framework
  efficient validation

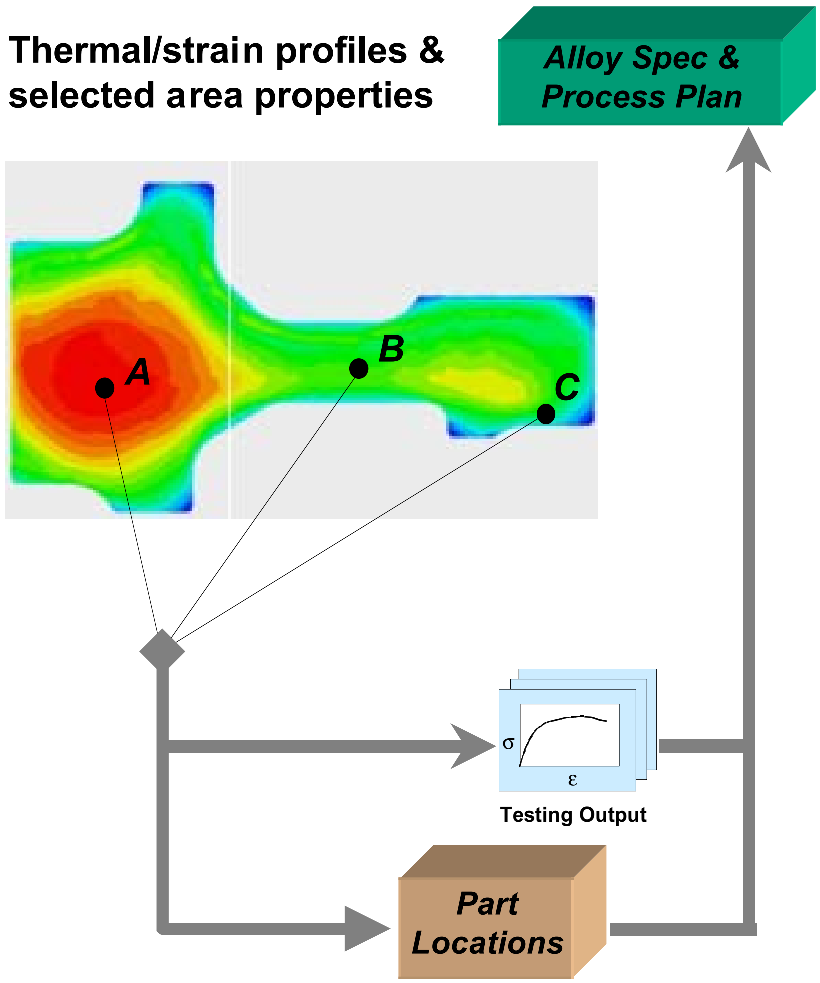
'Accelerated Insertion' Rather Than 'Materials by Design'

Modeling in the Component Design Process



"Field Experience" corrects for i) microstructure variation, ii) inaccurate analysis, & iii) incomplete understanding of service environment

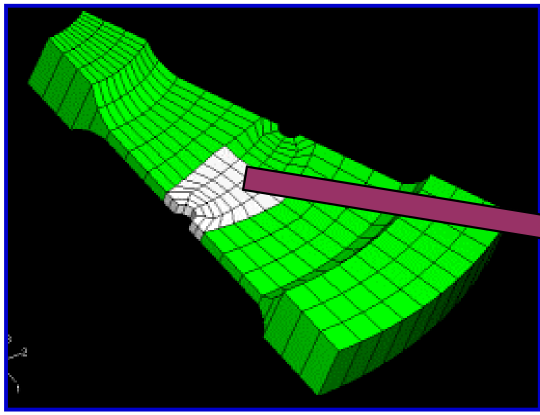
The Case of Ni-Alloy Engine Disks



- **Continuum codes (i.e., DEFORM) for thermal history and microstructure correlation over disk cross-section**
- **Cross-section may be "zoned" into a few regions (dual heat treat); *centimeter-scale homogenization***
- ***Empirical* yield-strength models, & flow-curve 'templates,' used to assign constitutive response**
- **Variation of structure averaged out; *local microstructure - defect interactions not represented***
- ***Data-intensive* and time-costly process for yield model and 'constitutive template' validation**

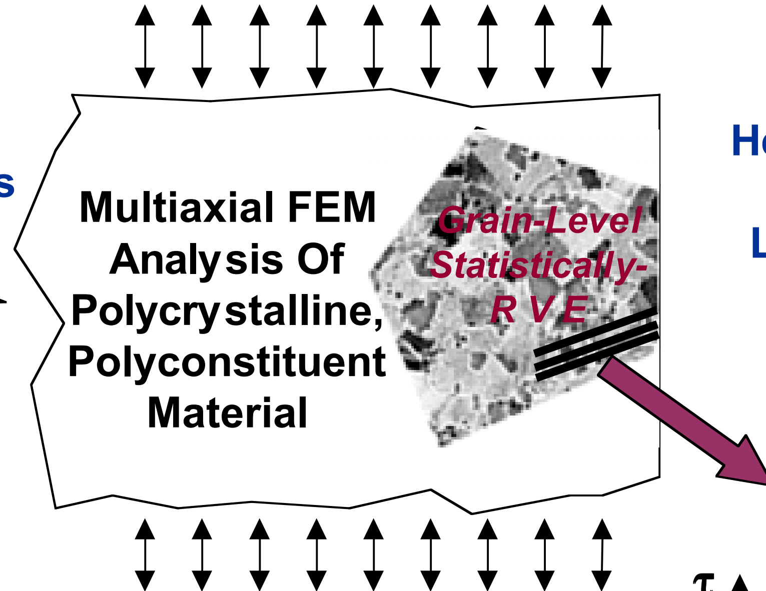
Challenges to represent time-dependent failure; to introduce "new material"

The “Plasticity Engine” for Properties

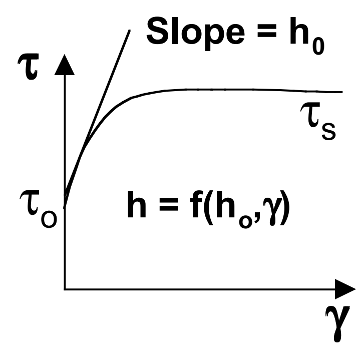


Design Concept

Define Features



Plastic Heterogeneity & Strain Localization



Properties of Representative Volume Element

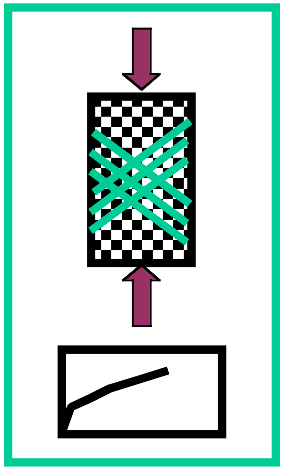
Focus on Work-Hardening Parameterization *With μ/s Effects*

$$\dot{\tau} = \left\{ h - \left(\frac{\tau - \tau_o}{\tau_s - \tau_o} \right) h \right\} \left(\dot{\gamma} / \dot{\gamma}_o \right)^m$$

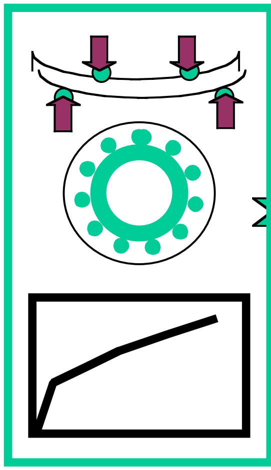
Conventional Finite Element Model	$\{\tau_o, \tau_s, m, h\}$
Continuum Crystal Plasticity	$\{\tau_{o,i}, \tau_{s,i}, m, h_{ij}\}$
Constrained Crystal Plasticity	$\{\tau_{o,i}(k_{hp}), \tau_{s,i}, m, h_{ij}\}$
Strain-Gradient Crystal Plasticity *must define τ (ρ), ρ (γ) to find k_o*	$\{\tau_{o,i}, \tau_{s,i}, m, h_{ij}\} + k_o$

increasing granularity & compute complexity

Build from Uni- / Multiaxial Slip & Work Hardening



uniaxial,
crystal test



multiaxial,
gradient test

Microstrain Experiments

**for single-, poly- &
polycrystalline slip**

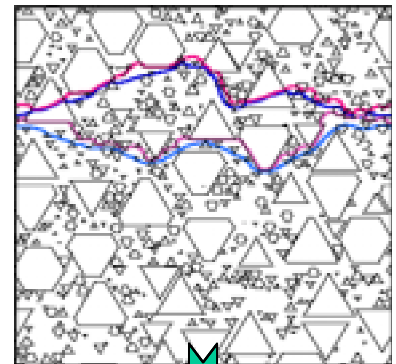
Microstructure Representation

characterize precipitate shape parameter and size/spacing distribution, etc.

Compare

Dislocation Kinetics Simulations

Intrinsic length effects, strain gradients



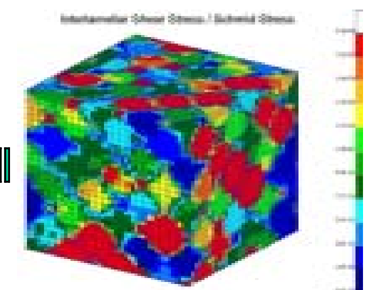
Existing links too weak

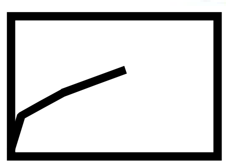
Numerical/Analytical Model

Representation of work-hardening from microstructure variation

~ <10 μm^3, 3-D

Scientific Frontier





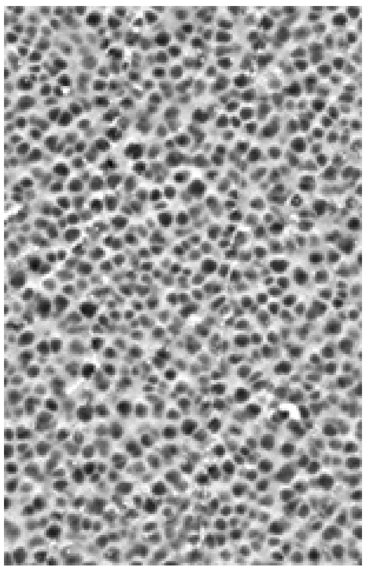
Predicted RVE Response

Single-slip & latent-hardening constitutive law for single-crystals; constitutive laws for polycrystalline RVEs (UMATs for 'intrinsic material' RVEs)

Direct links: computationally challenging & underdeveloped

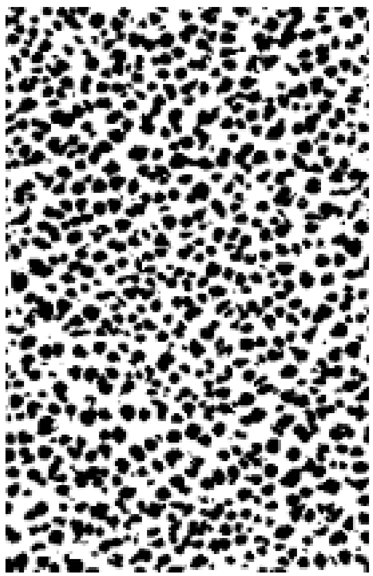
Real Microstructure in Simulations

TIFF
Image (PC)



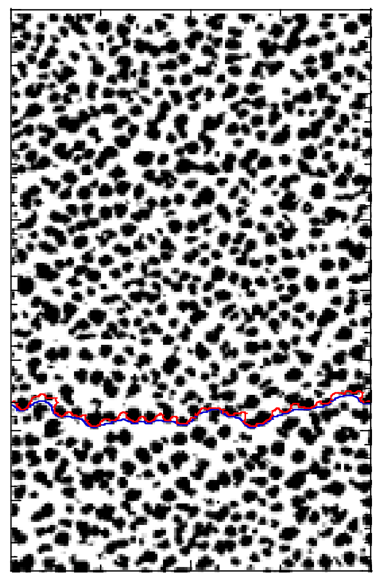
Rene88DT-Bore
2.5 x 4 µm
(BEI - S. Menon)

Binary
Image
(PC)

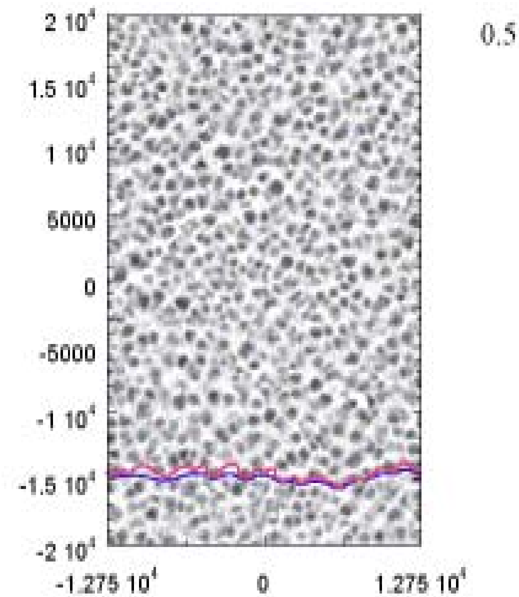


Simulation (Unix)
(pseudo-periodic)

τ =290 MPa



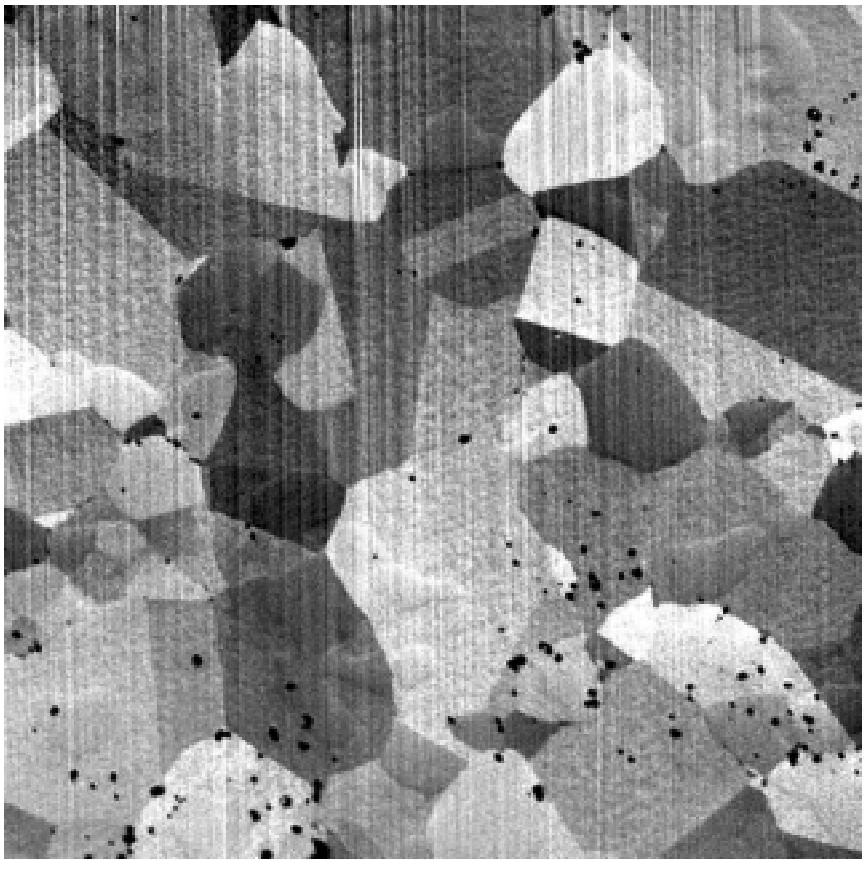
Simulation
superposed on
Microstructure



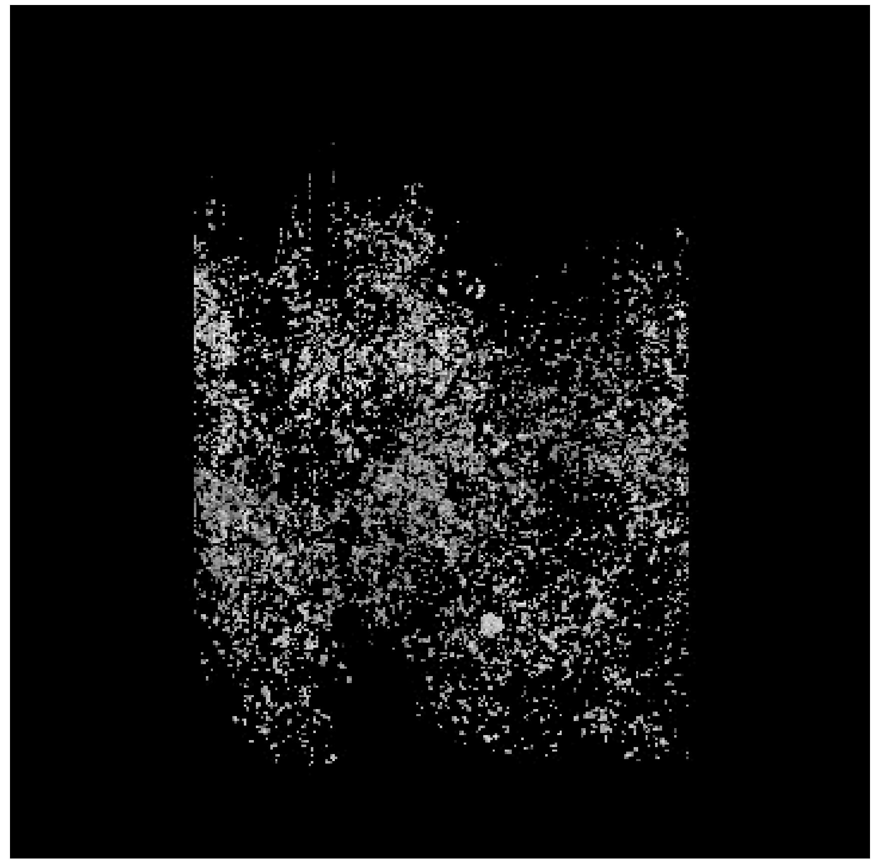
τ =290 MPa

3-D Quantitative Microscopy

Serial Sectioning & Imaging



3-D Rendering of Structure

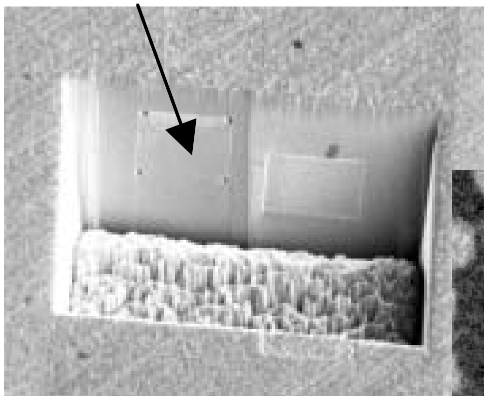


IN-100 Ni-base Superalloy
Grain Structure and Carbide/Boride Distribution

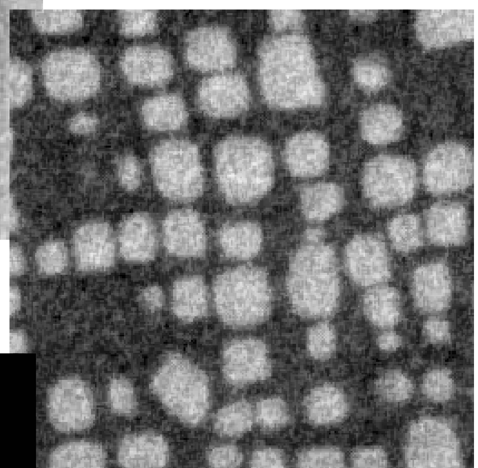
3-D Quantitative Microscopy

Serial Sectioning & Imaging

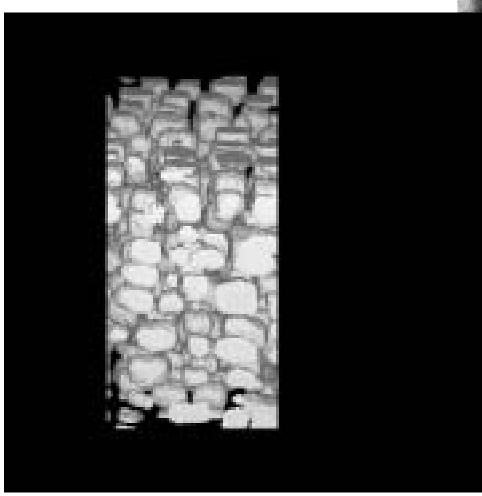
14 x 14 µm Image Area



Ni-Cr-Al Superalloy



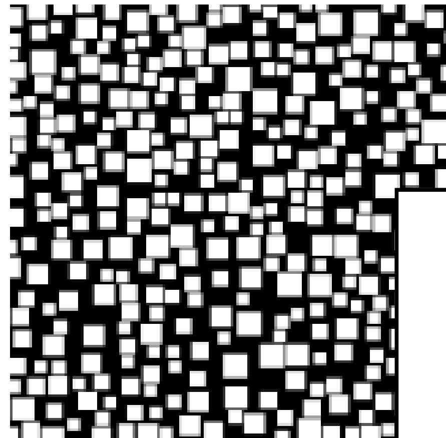
Aligned stack (~20 nm spacing)

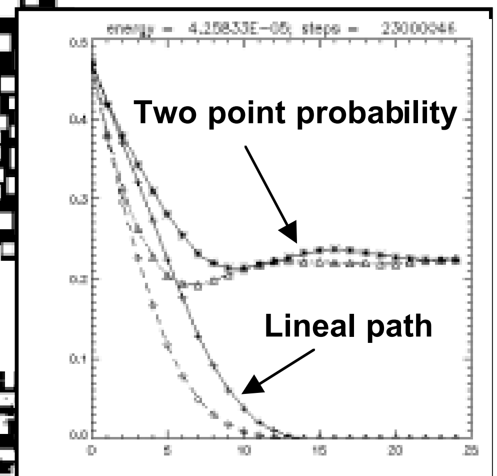


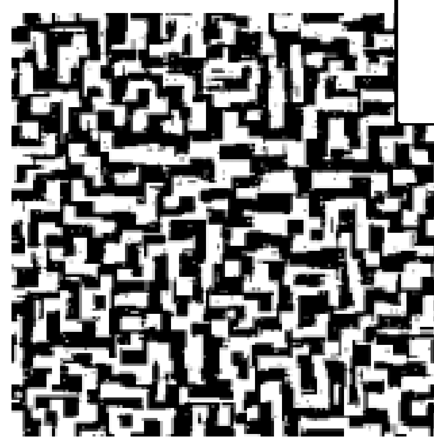
Rendered 3-D volume (~3 µm thick)

Mathematical Representation

Idealized Microstructure

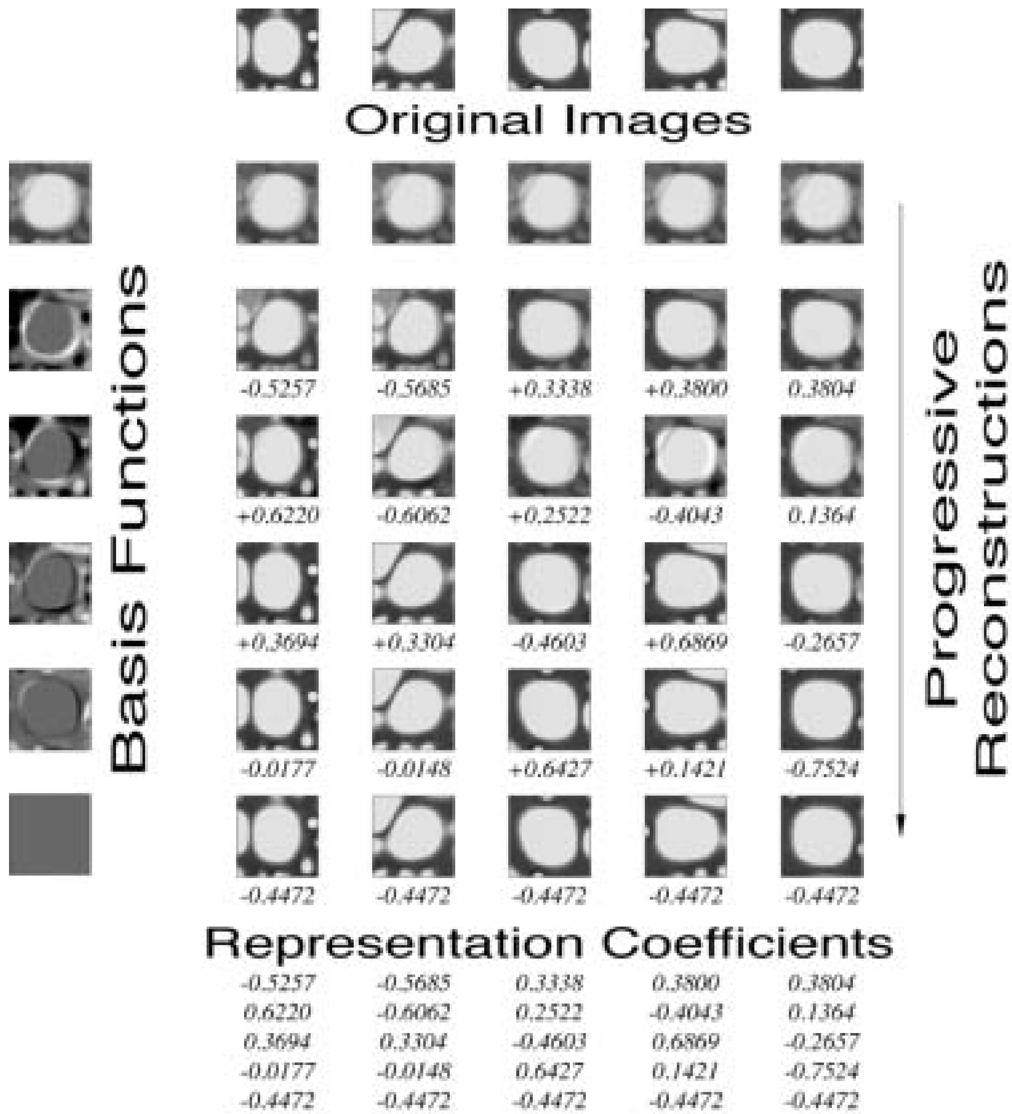






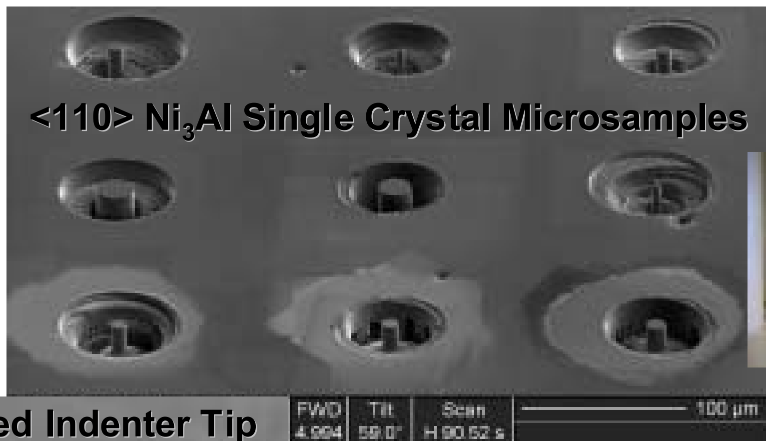
Monte Carlo Reconstructed Representative Microstructure

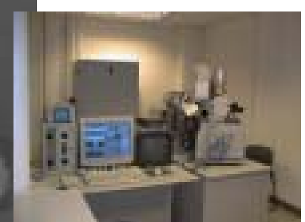
Principal Component Analysis of Microstructure



Mechanical Testing of Ultra-Small Samples for Crystal Properties

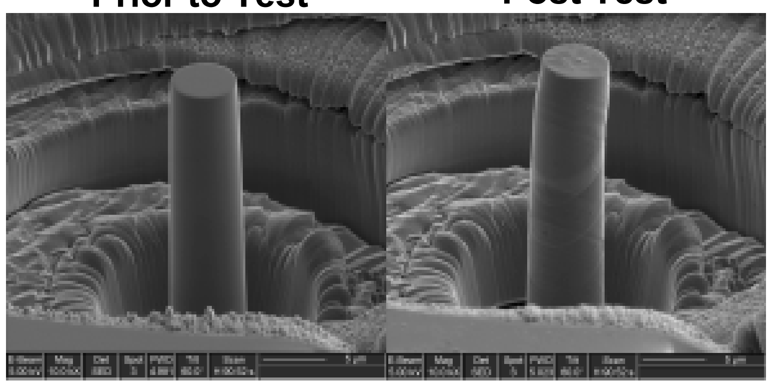
- *Focus efforts on linking simulation to design*
- *Small-scale properties measurement for constitutive representations*
- *Theory for broad understanding of deformation at small scales*

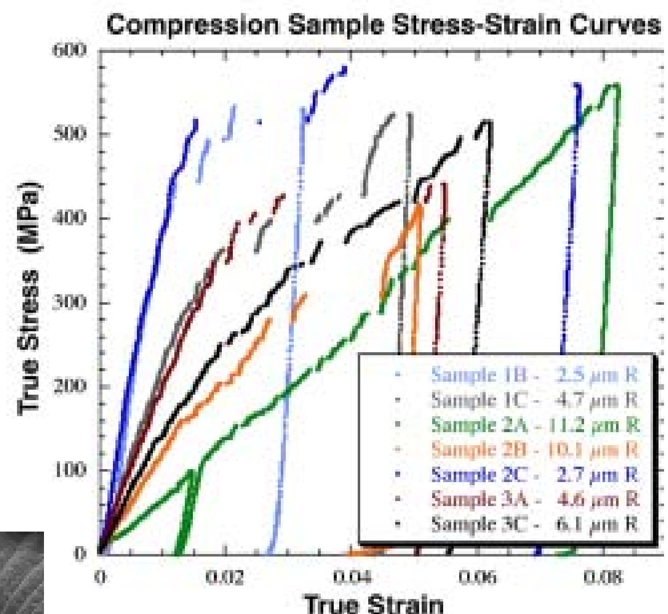




Prior to Test

Post Test

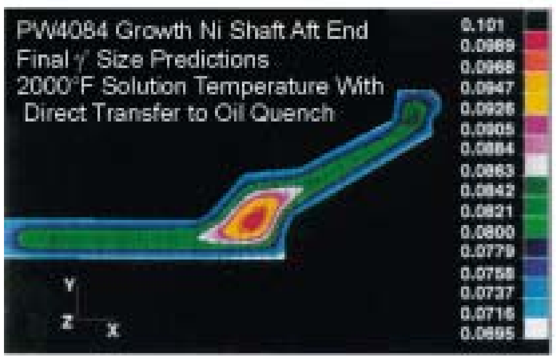


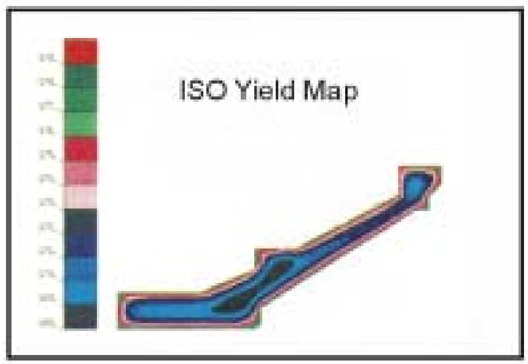


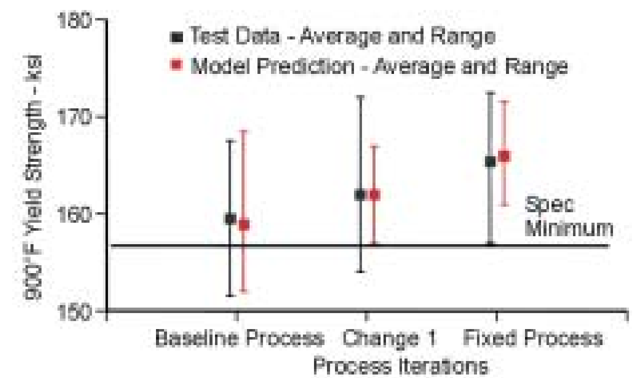
 Uchic, Dimiduk, Florando & Nix, 2002

Even Simple Models Have a Big Impact

- **Integrated structure-property-process models successfully applied as point solutions**
  - **statistically fit data to mechanistic-based property model**
  - **focused experiments to model microstructural evolution**
  - **accurate estimate of *mean* behavior**







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P & W →

Shaft design:
- 1/4 development time
- 80% reduction in cost

Experience shows concept is sound, projected payoffs reasonable

Eventually Must Address Full Breadth of Component Requirements

Requirements for Turbine Engine Disks:

- *Ultimate Tensile Strength*
- *0.2 % Yield Strength*
- *Tensile Ductilities*
- *Notch Strength*
- *Burst Margin*
- *Creep*
- *Rupture*
- *Rupture Ductilities*
- Continuous Cycling LCF
- Hold Time LCF
- Continuous Cycling Crack Growth
- Hold Time Crack Growth
- Superplasticity
- Flow Stresses
- Abnormal Grain Growth Resistance
- Gamma Prime Solvus
- Carbide(s) Solvus
- Density

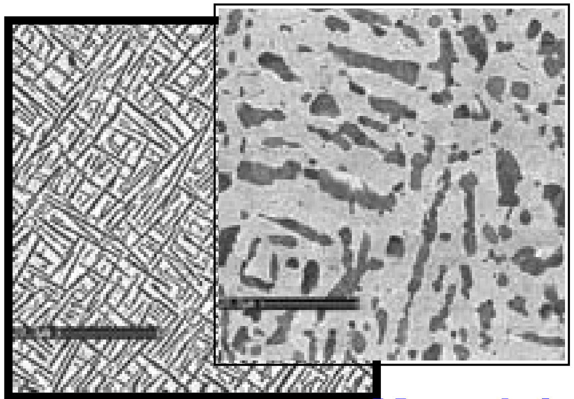
DARPA - AIM

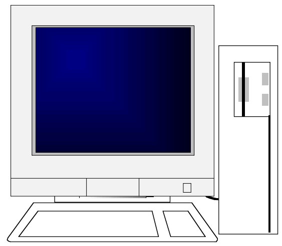
- TIP
- Structural Stability
- Exposed Behavior
- Defect Sensitivity
- Defect Content
- Grain Size
- Gamma Prime Size
- Segregation /Effects
- *Inspectibility*
- *Quench Crack Resistance*
- *Multi-source Capability*
- *Low Costs--Elemental and Processing*
- *Weldability*
- *Machinability*
- *Machined Surface Behavior*
- *Residual Stresses*
- *Cost Reduction Potential*
- *Size/Volume Scaling Effects*

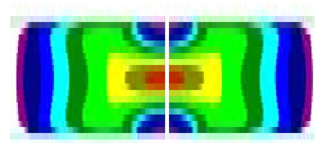
The Issues That Often Determine Success or Failure

Materials & System Readiness

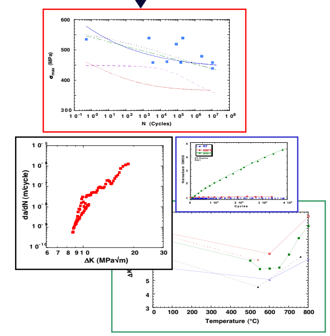
AIM







Materials Mathematics Experiment Experience



Property Database

Mathematics

State Awareness

Failure Physics

Data Fusion

Reasoning System

Prognostics

Combat System Readiness

Summary

- **The *time* for structural materials development and use must be shortened (time focus, not cost focus)**
- **Industrial M & P community demanding a quantum-leap in *relevant engineering simulation* capability**
- ***Accelerated Insertion of Materials* is the long-term, strategically-relevant, computational materials science & engineering vision**
- **Materials Science & Engineering community must produce *integrated predictive tools***
- **Accelerated insertion demands *integration of* engineering *design with M & P* to achieve true systems engineering of materials technologies**